Design of Selective Inhibitors for ARTD10 in an Interdisciplinary Approach

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The enzyme ARTD10 is a member of the ADP-ribosyltransferase family (ARTDs) and performs mono-ADP-ribosylation (MARylation).[1,2] In this post-translational modification it transfers the ADP-ribose moiety of NAD^+ on substrate proteins. Since ARTD10 participates in DNA repair, intracellular signaling and interacts with cMyc, it became a target of inhibitor development in the last years.[3,4,5] In general, most ARTD inhibitors are derived from the unselective inhibitor 3-aminobenzamide.[6,7] For example, the inhibitor OUL35, which is selective for ARTD10 and in the focus of our research, consists of two benzamide parts.[8]

Here we present the results of *in silico*, *in vitro* and *in cell* experiments on potential ARTD10 inhibitors. Furthermore, we draw a comparison between our suggested ARTD10 inhibitors and OUL35. Overall, we show how computational, organic and biochemistry can work together for the development and the characterization of potential inhibitors for ARTD10.

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